

# REPORT DOCUMENTATION PAGE

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Funding received from the Defense University Research Instrumentation Program (DURIP) was received and used to purchase an OPO laser system and its accessories. The system includes a Nd:YAG laser, the optical parametric oscillator, a frequency doubling system, a laser table and a pulsed wavemeter for wavelength calibration. This system has been installed in the laboratory, tested, interfaced via new computer programs to other equipment in the lab and used in initial experiments. The new system holds much promise to enhance research in gas phase metal complexes sponsored by AFOSR.			
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**- Final Technical Report -**

**Optical Parametric Oscillator System for Metal Cluster  
Spectroscopy**

**Defense University Research Instrumentation Program (DURIP)**

**For the Period July 1, 1997 to December 31, 1997**

**AFOSR Contract No. F49620-97-1-0122**

**Associated with AFOSR Contract No. F49620-97-1-042**

**“Structure and Dynamics in Metal-Containing Clusters”**

**June 1998**

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## OBJECTIVES

This instrumentation grant was awarded under the "DURIP" program for an Optical Parametric Oscillator (OPO) Spectroscopy System. The primary objective of this equipment grant was to purchase the OPO system and its accessories, to install it in the laboratory and to integrate it into existing AFOSR-sponsored research programs.

The OPO laser system includes a Nd:YAG pump laser, the OPO, a frequency doubler, a small laser table and a pulsed wavemeter for wavelength analysis and calibration. This state-of-the-art OPO system provides high energy pulsed laser light in the wavelength region of 225-1680 nm with narrow linewidth ( $0.1 \text{ cm}^{-1}$ ). The broad wavelength coverage is provided by a solid state device, eliminating the need for dye lasers and their associated disadvantages of multiple dye solution changes and waste solvent generation. Additional items in this system include a breadboard-type optical table for the OPO and a pulsed wavemeter device for accurate wavelength calibration.

This powerful spectroscopy system is required for ongoing work in the spectroscopy and reaction dynamics of metal containing clusters. Two important areas of investigation are underway which require broadly tunable lasers: 1) electronic spectroscopy and photodissociation of gas phase metal compound clusters and 2) electronic spectroscopy of progressively solvated metal atoms. In both areas, the research goal is to characterize new classes of molecules whose electronic spectra have never been investigated before and which are intractable for present theoretical methods. There is therefore no previous information about electronic states or spectra, and theoretical calculations cannot provide even a rough estimate for these energetics.

Spectroscopic searches therefore require long wavelength scans throughout the visible and ultraviolet wavelength regions. Prior to the purchase of the OPO system, the only option for these experiments was the use of dye lasers, but long scans require multiple dye solution changes, which are extremely inconvenient. The OPO laser system makes long wavelength scans far more convenient, and makes it possible to extend these experiments into the near infrared region where dye lasers do not operate. The OPO system provides a powerful spectroscopy system enabling and facilitating many new experiments in the spectroscopy and dynamics of metal clusters, which impacts on Air Force research priorities in atmospheric chemistry, new ceramic materials and solvation dynamics.

#### **STATUS OF EFFORT**

The OPO system was purchased from Continuum, Inc. It consists of a model 9010 Nd:YAG laser equipped with injection seeding, the "SunLite" OPO system, a frequency doubling system and the computer control for the device. This integrated system has superior performance, technical support and warranty compared to the comparable Spectra Physics system. The breadboard-type laser table was purchased from Newport Corporation, and the pulsed wavemeter was purchased from Burleigh (model WA-4500). Although these various items were ordered as soon as the DURIP award money reached campus, there were expected delays in delivery for these non-stock items. The last of these items arrived and were completely installed in our new renovated lab space in January 1998.

During installation, the PI and his graduate students received 2-3 days of on-site training in the operation of the OPO system operation. The next few weeks were spent in further training and testing in the operation of this new device, and new software was written to interface the scanning operation of the OPO with data acquisition from our molecular beam experiments. The system was fully operational together with the molecular beam experiments by about March 1998. The OPO system has been used independently to reproduce experiments previously performed with dye lasers, and it has been used in new experiments both alone and in combination with a dye laser (double-resonance experiments).

## ACCOMPLISHMENTS/NEW FINDINGS

The primary effort involving the OPO system in the last few months has focused on the spectroscopy of mass-selected metal ion complexes. Two specific systems have been studied,  $\text{Ca}^+$ -acetylene and  $\text{Mg}^+$ -Ne. In both cases, the metal ion complexes are produced by laser vaporization in a pulsed nozzle cluster source and detected with a reflectron time-of-flight mass spectrometer (RTOF). Complexes are mass selected with the RTOF instrument and photodissociated on resonance with excited electronic states. Detection of the  $\text{M}^+$  photofragment as a function of the excitation laser wavelength produces a photodissociation action spectrum. The electronic band systems correlate to the metal  $^2\text{P} \leftarrow ^2\text{S}$  atomic resonance, and the transitions are strongly allowed. The excited states probed are bound states with sharp vibrational and rotational structure; dissociation occurs by absorption of a second photon which carries the system to higher electronic

states. In both complexes, we observe progressions in the metal-ligand stretching vibration and we observe rotationally resolved band contours. These data confirm that the  $\text{Ca}^+ \text{-} \text{C}_2\text{H}_2$  species is a  $\pi$  complex with  $\text{C}_{2v}$  symmetry and a metal-acetylene bond distance of 2.80 Å. The  $\text{Mg}^+ \text{-} \text{Ne}$  data is also vibrationally and rotationally resolved, but the data is not completely analyzed as of this writing.

We anticipate that the OPO system will further benefit our lab as we extend spectroscopic capability into the infrared region of the spectrum and as we perform long searches for new spectra. Broad spectra, such as those expected for multiply solvated metal ions, will benefit from the smooth output energy over broad energy regions. The initial success of the OPO system is quite promising, and we expect significant progress over the next few years as we continue to use this powerful new device.

#### **PERSONNEL SUPPORTED BY AND/OR ASSOCIATED WITH PROJECT**

##### **Faculty:**

Professor Michael A. Duncan, PI

##### **Graduate Students:**

Student	Degree Program	
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Steve Pullins	Ph.D.	PII Redacted	
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John Reddic	Ph.D.	PII Redacted	
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John Buchanan	M.S.	PII Redacted	
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## PUBLICATIONS IN THIS FUNDING PERIOD

1. M.R. France, S.H. Pullins and M.A. Duncan, "Photodissociation Spectroscopy of  $\text{Ca}^+ \text{-C}_2\text{H}_2$  and  $\text{Ca}^+ \text{-C}_2\text{D}_2$   $\pi$ -Complexes," *J. Chem. Phys.*, to be submitted.
2. J.E. Reddic and M.A. Duncan, "Photodissociation Spectroscopy of  $\text{Mg}^+ \text{-Ne}$ ," *J. Chem. Phys.*, to be submitted.

## INTERACTIONS/TRANSITIONS

I visited the Air Force Geophysics Laboratory on March 9, 1998 and spent the day visiting the atmospheric chemistry and ion chemistry research groups. I visited labs and spent time with Drs. Rainer Dressler, Edmund Murad, Al Viggiano, Susan Arnold, Skip Williams and Steve Lipson. I presented a seminar on my AFOSR sponsored research entitled: "Spectroscopy and Dynamics In Novel Metal Containing Clusters."

### a) PRESENTATIONS

#### Invited Lectures Presented on this Research

1. "Photodissociation of Size Selected Metal Clusters in the Gas Phase," *Physical Chemistry Seminar*, University of California-Santa Barbara, January 1998.
2. "Spectroscopy and Dynamics In Novel Metal Containing Clusters," *Physical Chemistry Seminar*, University of Pennsylvania, February 1998.
3. "Spectroscopy and Dynamics In Novel Metal Containing Clusters," *Physical Chemistry Seminar*, Massachusetts Institute of Technology, March 1998.

#### Poster and Contributed Presentations of this Research

None

### b) CONSULTATIVE AND ADVISORY FUNCTIONS

None

### c) TRANSITIONS

None

**NEW DISCOVERIES, INVENTIONS OR PATENT DISCLOSURES**

None

**HONORS/AWARDS**

None